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RECENT DEVELOPMENTS IN ASSESSING MICROSTRUCTURE-SENSITIVE EARLY STAGE FATIGUE OF POLYCRYSTALS (POSTPRINT)

William D. Musinski
AFRL/RXCM

Gustavo M. Castelluccio
Woodruff School of Mechanical Engineering, Georgia Institute of Technology

David L. McDowell
School of Materials Science & Engineering, Georgia Institute of Technology

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6. AUTHOR(S)

William D. Musinski

Gustavo M. Castelluccio

David L. McDowell

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)

AFRL/RXCM
Air Force Research Laboratory
Materials and Manufacturing Directorate
Wright-Patterson Air Force Base, OH 45433-7750

Woodruff School of Mechanical Engineering
Georgia Institute of Technology
Atlanta, GA 30332

School of Materials Science & Engineering
Georgia Institute of Technology
Atlanta, GA 30332

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Recent developments in assessing microstructure-sensitive early stage fatigue of polycrystals

Gustavo M. Castelluccio [a], William D. Musinski [a,c], David L. McDowell [a,b,*]

[a] Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA 30332, USA
[b] School of Materials Science & Engineering, Georgia Institute of Technology, Atlanta, GA 30332, USA
[c] Materials and Manufacturing Directorate, Air Force Research Laboratory, Wright-Patterson AFB, OH, USA

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Fatigue failure is a leading concern for many applications involving structures for transportation, manufacturing, medical devices, and electronic components. Recent advances in modeling and simulation, coupled with in situ experimental techniques, have enhanced the understanding required to distinguish and characterize mechanisms of fatigue crack formation and early growth at scales of underlying microstructure. In particular, microstructure substantially influences high cycle fatigue resistance and contributes to variability of the fatigue response. This paper reviews the confluence of recent experimental and modeling advances aimed at understanding and modeling of the formation and early growth of fatigue cracks with size on the order of dominant microstructure attributes.

1. Introduction: the need for microstructure-sensitive modeling

It is well documented that microstructure has a dominant influence in the early stages of fatigue crack formation and growth, especially at low strain amplitudes, and contributes significantly to variability and minimum fatigue lives among a population of specimens. However, physically-based models for small fatigue cracks are still in their infancy. Indeed, we can envision approaches that will include the microstructure as a design variable for fatigue resistance [1,2].

This review focuses on recent advances in the assessment of the influence of microstructure on fatigue resistance. Hierarchical approaches have become popular to describe the behavior of fatigue cracks at different stages of development, typically demarcated in terms of crack length relative to microstructure scale(s). Focusing on progress over the past five years, we first address some relevant experimental studies for formation and early growth of microstructurally small cracks (MSCs) in fatigue. Such cracks are defined as having all dimensions (including the cyclic plastic zone and damage process zone) on the order of the spacing of dominant microstructure obstacles to growth, such as high angle grain or phase boundaries. We highlight the importance of such experiments in supporting models and present an overview of advances in modeling and simulation strategies. The paper concludes with a discussion of future experimental and modeling research priorities that may have the greatest impact on new understanding and practice in addressing the role of microstructure in fatigue.

2. Experimental studies of microstructure scale fatigue processes

2.1. Plastic strain localization and fatigue crack formation

The process of fatigue crack formation involves the localization of irreversible plastic strain within slip bands that normally forms intrusions/extrusions at surface grains or impinges on grain boundaries for non-surface grains. Through continued cyclic loading, these slip band mechanisms build up a sufficient degree of lattice/interface disruption to form a crack, whether of transgranular or intergranular nature. We employ the term fatigue crack "formation" rather than "nucleation" to refer to the processes by which a crack is manifested at the scale of individual grains/phases in cyclically deformed materials. This definition may combine elements of classical pre-and post-critical embryonic nucleation, along with limited crack growth in the initial nucleant grain/phase. The more commonly used term "crack initiation" refers to the combined processes of crack formation and growth to some predefined crack length that involves a typically large number of grains/phases, as is commonly employed in engineering practice.

* Corresponding author at: Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA 30332, USA.

E-mail addresses: david.mcdowell@mse.gatech.edu, david.mcdowell@me.gatech.edu (D.L. McDowell).

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Recent advances have coupled electron backscatter diffraction (EBSD) and scanning electron microscopy (SEM) techniques to characterize fatigue crack formation in relation to grain size, crystallographic orientation, and nearest neighbor grain interactions. Miao and coworkers [3] studied annealing twins and the cooperation among "microstructural arrangements" in Ni-base superalloy Rene' 88DT. They observed crack formation along favorably-oriented Σ_3 twin boundaries in surface grains having a size larger than three times the mean grain size; moreover, most fatigue cracks formed in clusters of grains having low misorientation. Similarly, Mu et al. [4] characterized the formation of slip bands in stainless steel 316L as a function of the Schmid factor and the slip planes that maximize the extruded volume from slip bands. These results reinforce the importance of considering effects of grain size and crystallographic orientation in MSC formation.

The digital image correlation (DIC) technique has been recently employed in conjunction with EBSD to explore the local, grain scale microstructure environments in which fatigue cracks form. Abuzaid et al. [5,6] employed high resolution DIC and EBSD to measure subgrain level surface strain and correlate the localization of plastic strain with microcracks in Ni-base superalloy Hastelloy X. Their results revealed that grain boundaries and twin interfaces (blocking or transmitting) differed in terms of behavior, and quantified a residual Burgers vector associated with the dislocation transmission process; such interface mediation of dislocations can strongly affect formation of fatigue cracks. El Bartali et al. [7] quantified plastic strain at the grain scale in a duplex stainless steel and measured a high degree of strain heterogeneity within some grains, attributed to local constraint and resulting triaxiality. Daly and coworkers [8–10] coupled DIC methodologies with infrared thermography and stereo digital imaging to characterize the behavior of shape memory alloys with resolution on the order of several microns. DIC has become an important validation tool for grain scale crystal plasticity models, but it still has its challenges, including the resolution necessary to resolve fine slip band structures and high-intensity illumination, heat haze and degradation of the speckle pattern at high temperature.

Highly detailed observations of formation and growth of fatigue cracks from free surfaces are facilitated using in situ loading stages [11] with microscale specimens and MEMS devices [12,13]. These techniques have characterized early stage fatigue damage at the micron scale arising from grain-to-grain incompatibility, as well as degradation of coatings and oxides. Surface topology/roughness has been studied as an indirect measure of the local irreversibility. Ho et al. [14,15] assessed the influence of precipitates and grain size on extrusion height in a Ni-base superalloy to conclude that the critical extrusion height (the average extrusion height from damaged grains) depends on grain size; the degree of plastic strain localization within bands does not. El Bartali et al. [16] compared the wavy versus planar slip topology in ferritic and austenitic grains in duplex steels with resolution down to the nanometer range using interferometric profilometry. SEM and Focused Ion Beam (FIB) sectioning techniques [17–20] have been employed to characterize mesoscale dislocation arrays, slip transmission, intrusions and extrusions, orientation and early growth of small fatigue cracks. Other efforts [21,22] have combined techniques to study the effects of hydrogen on strain localization and have quantified the slip band spacing in hydrogen-charged specimens; this points to the importance of considering environmental effects in constitutive models framed at the scale of microstructure, in addition to effects on crack tip slip irreversibility that controls fatigue crack growth.

2.2. Growth of microstructurally small fatigue cracks

An increasing range of experimental techniques is being introduced and developed to assess the propagation of cracks with size on the order of microstructure scale. Marking of the crack front at a given number of cycles by applying periodic blocks of "underload" cycles [23,24] has successfully facilitated estimation of MSC contours over several grains. This technique is limited to material systems that display different deformation behaviors at low versus high strain amplitudes (e.g., aluminum alloys) and the crack front can only be marked after a certain number of cycles, which limits the resolution of the inferred crack growth rate. It may have somewhat more applicability to modeling growth of long cracks rather than MSCs.

Other methods used to monitor 3D evolution of MSCs at the grain scale include high energy X-ray diffraction microscopy (HEDM) and X-ray diffraction contrast tomography (DCT), also known as microCT (μCT) [25,26]. HEDM non-destructively maps the microstructure (grain size and morphology, crystal orientation, etc.), while DCT monitors the evolution of cracks or voids. Multiple researchers have monitored in situ microstructure evolution and 3D crack growth using this method for a wide variety of materials (cf. extensive review by Stock [27]). In recent work [25,26,28], FIB notches comprising a few grains were used to promote formation of fatigue cracks under constant amplitude loading and with overloads; by continuously cycling and imaging, researchers have been able to characterize the fully 3D evolution of the crack front and crack tip opening displacements within the bulk of the material throughout the fatigue process. Liu et al. [29] employed synchrotron X-radiation to image naturally occurring 3D fatigue crack formation in Ni base superalloy single crystals, and characterized the interactions between the crack front and local microstructure. HEDM can also be used at high temperatures ($\sim$1750 °C) [30] at high spatial resolution, which can facilitate the study of MSCs under thermomechanical fatigue.

X-ray tomography has been used to characterize the initial size and morphology of grains and defects, followed by post-test characterization (SEM, serial sectioning, EBSD, etc.) to further validate sites of fatigue crack formation and early growth. For example, Nicoletto et al. [31] used X-ray tomography to characterize the extreme value distribution of pore shapes and sizes relevant to cast $AlSi_7Mg$ specimens. Their finite element (FE) work highlighted the importance of morphological stress concentration induced by the irregular-shaped pores prevalent in this microstructure as opposed to simply considering pores as equivalent spherical or ellipsoidal shapes. Likewise, Vanderesse et al. [32] used X-ray microtomography to study the effect of pores in a pressure die-cast aluminum alloy, $AlSi_9Cu_3$ (Fe); they found that the most detrimental defects were on the high end of the pore size distribution and cracks occurred in pore-rich regions.

The interaction between fatigue cracks and grain boundaries is also quite pertinent to MSC growth analysis and prediction. Caton et al. [33,34] assessed the role of dwell time and stress ratio on MSC growth in Ni-base (naturally occurring) and Ti alloys (small machined notches), respectively. Szczepanski and collaborators [35] employed micro-notches with length corresponding to several grain sizes in Ti alloys and deduced that the variability of MSC growth rates is much lower than the variability of total fatigue life; therefore, most variability is attributed to the process of forming and growing MSC cracks in very early stages. Marx and coworkers [36–39] performed novel studies on the effects of grain boundaries on Stage I (crystallographic) fatigue crack growth in a directionally-solidified CMSX-4 Ni-base superalloy by introducing FIB notches (30–60 μm, semi-circular) within selected surface grains, oriented along the slip system with the highest Schmid factor, attempting to mimic naturally occurring cracks. By measuring the crack length periodically via a replication technique, the authors quantified a decreasing crack growth rate as the crack approached a grain boundary. Additionally, the crack path was reconstructed via FIB serial sectioning to obtain slices on the order of

100 nm thickness (cf. Fig. 1); they found that cracks do not necessarily propagate into a neighboring grain along slip planes with the highest apparent Schmid factor, but rather along the most compatible slip plane (lowest tilt/twist angle), which is consistent with previous studies on an aluminum alloy by Zhai et al. [40]. Such results have rarely been considered in engineering models.

3. Modeling the influence of microstructure on fatigue

3.1. Plastic strain localization and fatigue crack formation

Tanaka and Mura [41] and Navarro and de los Rios [42] pioneered the application of distributed dislocation models to describe the growth rate and GB interactions of MSCs in fatigue. These distributed dislocation approaches are still being extended [43,44] and continue to influence modeling concepts for Stage I MSC growth. Dislocation dynamics (DD) investigations of fatigue response of complex alloys have been employed to study the formation of mesoscale dislocation structures; Vattré et al. [45] analyzed the interaction of dislocations with precipitates by suppressing or activating cross-slip and characterized the mechanisms that lead to slip localization, as shown in Fig. 2(a). Prasad Reddy et al. [46] used DD simulations to model plastic localization in grains that neighbor the crack front (Fig. 2(b)) for multiple tilt and twist angle configurations without slip transmission and showed that dislocation activity strongly depends on the stress field in the cracked grain; therefore, slip localization may not accord with Schmid's law. Hansson and Melin [47] employed DD in a boundary element framework to model slip transmission across a low angle grain boundary under cyclic loading and with overloads; grain boundaries were modeled as a wall of evenly spaced dislocations. Their results showed that development of dislocation pile-ups and MSC growth rates depend on the spacing among dislocations (i.e., low angle misorientation) that comprised the grain boundary, while overloads may or may not decrease crack growth rates.

Sangid and coworkers [48–52] developed an energy-based approach informed by atomistic simulations for modeling fatigue crack formation associated with PSB/matrix and PSB/GB interactions. A number of random polycrystalline aggregates were considered to predict the minimum number of cycles to form a fatigue crack, as well as the scatter of high cycle fatigue response. This formulation conceptually appeals to a ladder-type of dislocation arrangement that is well documented for pure Cu, for example, but may not be universally applicable to metal alloys.

Much remains to be explored regarding the interaction of plastic strain localization and microstructure attributes such as coherent precipitates, phases, twins and point defects, for example. Brown [53] reviewed the role of vacancies and interstitials in plastic strain localization. Polak and coworkers [54,55] extended earlier point defect diffusion schemes to model the temperature dependence of PSBs in accordance with experimental measurements. However, most point defect models assume the formation of ladder-type dislocation arrangements; the role of vacancies in fatigue crack formation in other cases such as low stacking fault energy materials, for example, has not been considered to the same extent. Moreover, the interaction between the environment and point defects, which influences the irreversibility within the crack tip process zone, is poorly understood and has not been substantially considered in fatigue modeling.

Kunkler et al. [56] and Kübbeler et al. [57] successfully employed a 2D boundary element method to model plastic localization MSC growth among multiple grains and Stage I–Stage II transition. Hilgendorff et al. [58] also employed 2D boundary element methods to model the slip band impingement on the grain boundary and shear stress fields within grains. These 2D studies reinforced the utility of cyclic crack tip displacement along with explicit consideration of the microstructure to model MSC growth, motivating extension of these methods and concepts to 3D MSCs.

Building on work since the late 1990s regarding explicit consideration of hierarchical microstructure in manifesting multiple stages of fatigue crack formation and growth, McDowell [59] and McDowell and Dunne [60] reviewed crystal plasticity-based multistage approaches for the assessment of fatigue of microstructures. Such approaches have considered fatigue crack formation and MSC growth, including consideration of detailed microstructure representation and dislocation-based deformation mechanisms, as well as growth of physically small fatigue cracks and transition to long crack growth behavior. For example, Zhang et al. [61] used a softening formulation for the primary alpha phase of Ti–6Al–4V along with distributed initial imperfections to facilitate slip band localization and cyclic softening in a 3D crystal plasticity model; the slip band thickness was imposed following experimental observations, while orientation and spacing were allowed to evolve in accordance with applied loading and constraints of the local microstructure environment. Bridier et al. [62] performed a study comparing relative levels of basal, prismatic and pyramidal slip system activation in Ti–6Al–4V using a crystal plasticity constitutive model, emphasizing the importance of slip system softening in the primary alpha phase of this particular alloy system associated with breakdown of short range order as the first dislocation passes through. Single slip was typically observed at low applied strain amplitudes, and fatigue cracks were associated with a combination of relatively high Schmid factor along with a tensile stress normal to the basal plane, which supports the use of slip band-based fatigue indicator parameters (FIPs), such as the Fatemi–Socie parameter [63].

Dunne and coworkers [64] performed a detailed comparison between experiments and crystal plasticity models to characterize

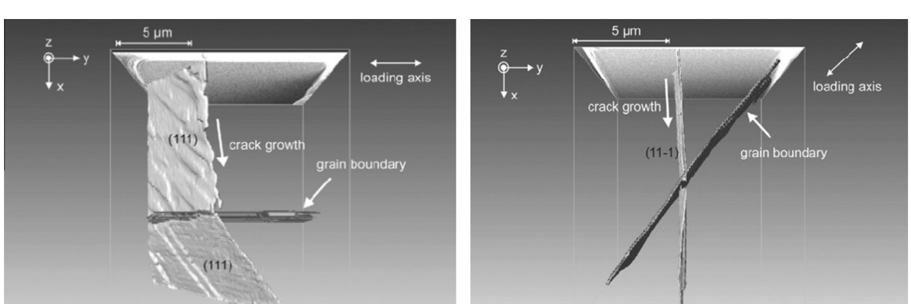

Fig. 1. Reconstruction of crack growth across a grain boundary using serial sectioning with FIB in CMSX-4 Ni-base superalloy. At left, the crack exhibited almost no retardation of the growth rate at the grain boundary, even when shifting its growth direction. At right, the crack penetrates directly through the grain boundary. In both cases, the crack formed and propagated along ⟨1 1 1⟩ planes. Reproduced from [36].

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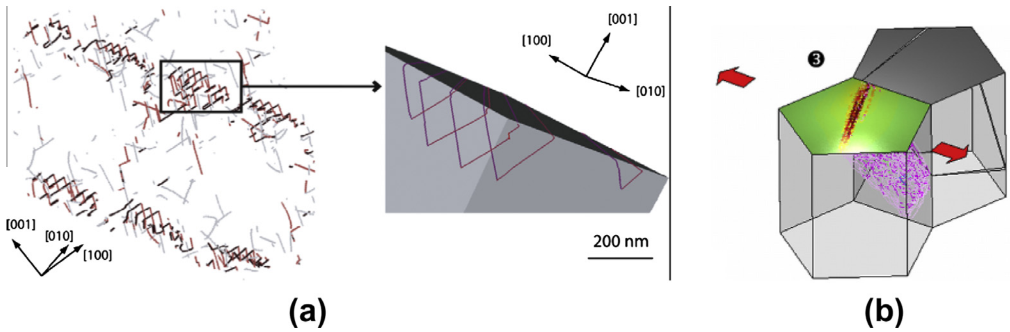

Fig. 2. (a) Simulated dislocation substructure in a matrix channel for the ⟨1 1 1⟩ loading case after 0.2% plastic strain accumulation [45] and (b) strain localization within a grain due to a crack in a neighboring grain [46].

crack formation in single edge four point bending specimens of a polycrystalline ferritic steel (Fig. 3); their model simulated the grain morphology and crystallographic orientation distribution at the notch root in specimens. They were able to predict the location of crack formation and suggested that effective plastic strain per cycle is a better indicator for the site of fatigue crack formation than cumulative effective plastic strain over many cycles. Li and coworkers [65,66] constructed microstructure aggregate finite element models for 304L stainless steel using EBSD measurements taken on successive slices of microstructure through the thickness. Their work simulated overload effects using a constitutive model calibrated with stress–strain hysteresis loops at mid-lives for multiple strain ranges, although overload transients were not considered. The overloads affected the stresses and strains on the surface elements, but the effects of overload were more significant for lower strain ranges.

Nonlocal FIPs have increasingly been used as mesoscopic indicators to relate to processes of fatigue crack formation and growth of MSCs. Littlewood [67] employed a nonlocal peridynamics modeling approach with crystal plasticity to compute a Fatemi–Socie-based FIP for single crystals. Ferrie and Sauzay [68] analyzed the effects of first nearest neighbor grains on crack tip opening and sliding displacements using a crystal plasticity model with elastic anisotropy. Their results showed that the crystallographic orientation of the nearest neighbor grains have a significant effect on cyclic crack tip displacement. Modeling single crystals with and without slip bands subjected to cyclic shear with and without superimposed cyclic normal stress to the crack plane, Castelluccio and McDowell [69] found an almost linear relation between the cyclic range of crack tip displacement and the nonlocal Fatemi–Socie FIP. Such a relation holds in the case of localized plasticity and supports the statistical assessment of fatigue resistance of different microstructures using FIPs [70]; it has been used to quantify the influence of twins in cyclic plastic shear strain localization and crack formation [71]. Hochhalter and coworkers [72,73] used crystal plasticity simulations to compare multiple 1D nonlocal FIPs in the neighborhood of inclusions in Al alloys. Their work highlighted the importance of considering the experimental variability when validating crack nucleation models. Their results also show that the selection of the FIP is as important as the domain over which it is computed; 1D domains may not be appropriate for 3D processes regardless the FIP formulation. Guilhem et al. [74] compared grain-averaged accumulated plasticity with several other FIPs using 2D crystal plasticity and concluded that the crystallographic orientation of second and third nearest neighbor grains from the surface grain under consideration influence the driving forces to form and grow MSCs. Ghosh and collaborators [75–78] developed a microstructure-sensitive fatigue model for Ti-alloys based on stress redistribution between adjacent hard and soft grains. Their criterion for fatigue crack formation is nonlocal, depending on effective stresses in the hard grain and the plastic strains and strain gradients in adjacent soft grains.

McDowell and coworkers pursued statistical approaches combined with 3D crystal plasticity models and nonlocal FIPs to quantify the variability of fatigue crack formation and early MSC growth. Przybyla and McDowell [79,80] simulated a large number of periodic statistical volume elements (SVEs) of realistic microstructure to capture the extreme values of driving forces for MSC formation (i.e., minimum lifetime) for Ni base superalloy IN100 [79] and dual phase Ti–6Al–4V [80]. Nonlocal maximum FIPs for all SVE samples were in accordance with the Gumbel extreme value distribution, enabling comparison of the minimum lifetime fatigue response among microstructures; marked spatial correlation functions (radial distribution functions) quantified the coupling of microstructure attributes (e.g., grain size, orientation, phases) in regions of high FIP values and established the likelihood for most detrimental features associated with MSC formation. Transition from surface to subsurface fatigue crack formation with a decrease in applied stress or strain amplitude has also been considered using this type of framework [81,82].

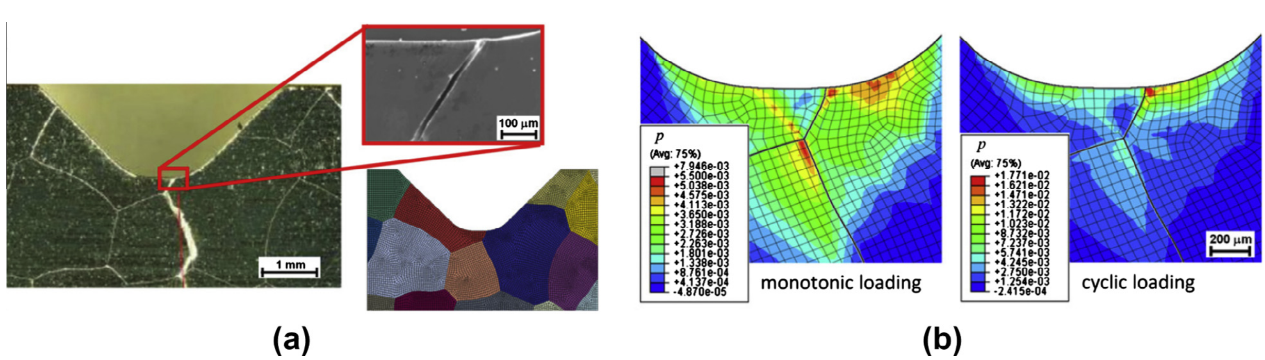

Fig. 3. Example of (a) the specimen notch and FE model and (b) monotonic and cyclic plasticity for a four-point bending experiment on a polycrystalline ferritic steel [64].

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Salajegheh and McDowell [83] introduced a probabilistic strategy to model the surface to bulk transition of high cycle fatigue crack formation associated with primary inclusions in IN 100 Ni-base superalloy. Prasannavenkatesan and co-workers [84,85] considered effects of shot peening-induced surface residual stresses, pores, and hard and soft primary inclusions in martensitic gear steel in the context of 3D polycrystal plasticity and nonlocal FIPs. Coupled effects of inclusion fracture/debonding and initial subsurface residual stress following carburization and tempering were considered as a function of surface proximity to estimate likelihood of depth of crack formation. They concluded that residual stress relaxation could only be modeled using polycrystal plasticity [86].

Owolabi et al. [87] developed a probabilistic methodology applied to the highly stressed volume of notches, along with a probabilistic mesomechanics approach to quantify notch size effects by defining a microstructure-sensitive fatigue notch factor that considers the probability distribution of the high cycle fatigue strength. The foregoing approaches for modeling formation of fatigue cracks are primarily useful for comparing microstructures in terms of fatigue resistance. Cyclic plastic strain localization and cracking processes occurring at the subgrain scale have relatively high uncertainty, which can be reduced in time via coupling with in situ experiments and bottom-up modeling and simulation.

3.2. Microstructurally small fatigue crack growth

Multiple finite element modeling efforts have explored the growth of MSCs with and without explicit provision for crack extension. Mikkola et al. [88] analyzed fatigue crack growth using an hexagonal 2D microstructure and an elastic–plastic model with deformation occurring along discrete planes. They computed the number of cycles to extend the crack up to the next grain boundary assuming that the plastic shear strain range increases linearly with the number of cycles and the stress and strain ranges remain constant within a grain (Miller–Hobson [86]); cracks extend along the slip system with the highest average resolved shear stress up to the first grain boundary. The results showed that the stresses in subsequent grains increase only marginally (between 10% and 20%) after crack advance through the first and second grains subsequent to crack formation. Kramberger and Jezernik [89,90] proposed a 2D elastic model that considers crack formation along slip bands within grains. The driving force for fatigue cracks within the grain is assessed by subdividing the slip bands into segments and computing the lives for each segment. The average shear stress range over the entire slip band decreased with increasing crack length, even though the shear stress averaged within the segment ahead of the crack tip tends to increase with crack length.

Castelluccio and McDowell [91] introduced 3D crystal plasticity models to assess the evolution of the Fatemi–Socie FIP averaged along crystallographic planes within grains; crack growth was considered via the reduction of the elastic stiffness in elements associated with the crack plane. As the cracks extended along crystallographic bands that span the entire grain cross section, the FIP decreased (Fig. 4), following a trend similar to the relation of Hobson et al. [92] as MSCs grow through several grains; this approach can predict the evolution within grains for a given microstructure instantiation. Castelluccio and McDowell [93] later employed the evolution of the FIP in a mesoscale approach to estimate the fatigue resistance of bimodal microstructures.

Musinski and McDowell [94] employed a 3D crystal plasticity FE model to assess the fatigue life scatter of notched specimens with different notch root radii sizes in random microstructures of equiaxed IN100 and predicted the number of cycles to propagate a MSC; the crack growth rate was assumed to be proportional to the value of Fatemi–Socie FIP assessed from simulations of

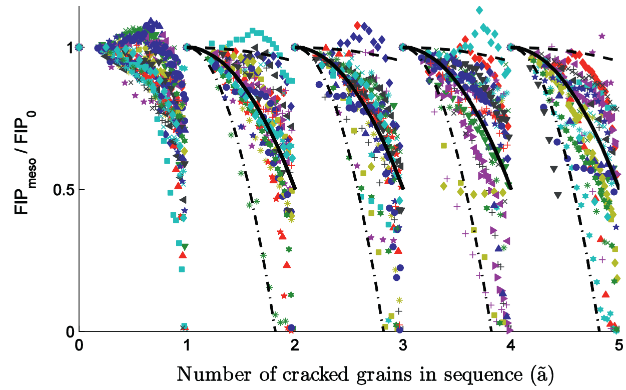

Fig. 4. Evolution of the nondimensionalized mesoscale FIP for crack extension within a grain [91]. FIP_0 refers to the FIP prior to cracking each individual grain, and $\tilde{a}$ is the cracked slip plane area fraction within each grain that effectively tracks number of grains involved in crack advance. The normalized FIP_{meso} decreases as the crack grows within grains along a predefined slip plane.

polycrystals without cracks, along with a crack length dependence proposed by Shenoy et al. [95]. A probabilistic approach based on a transition crack length for MSC growth from the notch root to long crack LEFM behavior was introduced to explore the fatigue life variability under HCF and VHCF conditions, and the results were characterized using a cumulative distribution function.

Crystal plasticity FE approaches have also been employed to quantify the influence of the microstructure on fretting fatigue. Dick and coworkers [96] analyzed driving forces and characterized fretting maps. Sadeghi and coworkers [97–100] introduced 3D FE simulations to study microstructure-scale fatigue crack growth in MEMS and fretting fatigue. Their methodology considers a mesh with duplicate nodes along the grain boundaries to account for crack growth with an elastic–plastic model invoking isotropic damage, which evolves with number of cycles for an applied stress range. These models were calibrated with experimental data to simulate the number of cycles to form a fatigue crack for multiple load ranges, and were used to assess the variability associated with multiple microstructural realizations. Bares et al. [101] employed cohesive elements to simulate thermomechanical fatigue crack formation and growth.

Osterstock et al. [102] combined FE simulations with estimation of the height of slip bands based on DD to model fatigue crack formation and growth through the first few grains. Crack formation was assumed to occur when the accumulated irreversible slip reached a critical value that was consistent with previous AFM measurements.

4. Discussion and conclusions

4.1. Impact of experimental techniques on microstructure-sensitive modeling

Enhanced capabilities offered by emergent experimental methods provide a myriad of opportunities to advance microstructure-sensitive fatigue modeling. Constitutive models for cyclic stress–strain behavior and fatigue crack growth models can be reformulated based on mesoscale cyclic strain calibrations and crack growth rates measured at the scale of microstructure, facilitating improvement of model forms and parameter validation. A strategy is required to extrapolate the deformation and failure mechanisms at the finest scales to length scales that are relevant to components and laboratory specimens. This also should consider the concept of a statistically-representative volume of microstructure, which relates more to component level fatigue life prediction and associated variability. The selection of mesoscale volume size in

simulations, typically considered as a statistical volume element rather than a representative volume element, should consider the physical length scales of nonlocal interactions among features of microstructure that influence fatigue crack formation and early MSC growth. Statistical variability can be understood on the basis of large numbers of such simulations or experimental specimens to incorporate aleatory uncertainty arising from randomness of microstructure.

In spite of advances in experimental methods, it is still difficult to study the behavior of naturally occurring fatigue cracks at very early stages of formation and growth. The experimental assessment of extrusions/intrusions has motivated advances in dislocation models that consider crack formation associated with the localized cyclic plasticity. Similarly, the assessment of the influence of the grain boundary network (e.g., tilt/twist, disorientation) on crack advance across grain boundaries is essential for physically-based MSC growth models. Notches at the scale of microstructure have often been introduced using FIB techniques, for example, as a means to guide the process of MSC growth in early stages for practical purposes of observation. However, such notches exclude the earlier stages of slip irreversibility and associated lattice distribution, and predetermine the initial shape and orientation of small cracks. Moreover, these approaches likely reduce the sensitivity of the fatigue crack growth rate on the microstructure and raise questions regarding the transferability and interpretation of growth rate measurements as crack fronts approach and cross grain boundaries. As a result, hierarchical modeling approaches require the calibration of different regimes using different experimental techniques, and the boundaries of each regime depend on the interplay of modeling constructs and experimental capabilities to quantify microstructure and discern failure mechanisms.

The implementation of microstructural-sensitive modeling strategies at an industrial scale is still a challenge, but several high-end applications have started exploring their benefits. Most notably, the design and/or development of fatigue-resistant microstructures [103] has received significant attention since the precise estimation of fatigue life is not as important as qualitative ranking of the relative fatigue resistance and variability among candidate variant microstructures. The implementation of microstructure-sensitive algorithms to support structural fatigue design in industry applications is still a challenge, particularly with regard to the multitude of aspects involved: experiments and characterization of microstructures, modeling at multiple scales, detailed description of loading conditions and environments, and prognosis of damage evolution in structures, among others. Mesoscale microstructure-sensitive modeling approaches provide a key opportunity for structural integrity assessment since they convey the information necessary to bridge the local and global field approaches, and can incorporate complex considerations such as materials processing and manufacturing.

4.2. Open areas for future research

Experimental techniques are evolving rapidly, and in many respects are outpacing the somewhat rudimentary modeling approaches used for MSCs, especially those based on variants of traditional LEFM that frame an effective driving force to describe MSC growth or focus on the equivalent initial flaw size concept to indirectly incorporate microstructure effects. Coupling advances in technologies related to in situ experiments with more physically-based modeling and simulation approaches offers multiple opportunities to deepen understanding of MSCs under fatigue loading. Non-exhaustively, these include:

- Measurement of local driving forces, such as localized cyclic plastic strain and cyclic crack tip displacement, and validation of microstructure-sensitive modeling strategies for most probable sites of fatigue crack formation and MSC growth path.
- Consideration of small 3D crack fronts in the subsurface, moving beyond surface measurements.
- Quantifying spatial distributions of crack lengths and fatigue crack growth variability in relation to the microstructure.
- Experiments that mimic and characterize naturally occurring small fatigue cracks to better quantify processes of MSC growth and interpretation in terms of mechanisms and behavior within the first few grains following crack formation, as well as transition to fully developed cracks amenable to more conventional fracture mechanics descriptions.
- Effects of environment and point defects, vacancies in particular, on fatigue crack formation and MSC growth.
- Standardization of metadata necessary to properly characterize initial and boundary conditions, as well as microstructure spatial correlations, to support microstructure-sensitive assessment.

Improvements in constitutive modeling strategies for subgrain scale cyclic plasticity (linking atomistics and discrete dislocation simulations to continuum crystal plasticity) are necessary to advance computational fatigue methodologies. These models should accord with the physics of mesoscale dislocation structures and should also reflect appropriate length scale effects and microstructure size dependence. This includes the influence of grain and twin boundaries on slip transfer of dislocations and crack tip irreversibility that governs the local crack growth rate. This is a major mesoscopic gap in the existing state-of-the-art. Other specific weaknesses to address in future modeling approaches include:

- A methodology for decomposition of stages of fatigue and associated mechanisms, including recognition of the limitations of conventional linear elastic and elastic–plastic fracture mechanics applied to small fatigue cracks.
- Feasible simulation strategies to consider transient evolution of stress and strain fields over many fatigue cycles, even for constant amplitude loading. Complexities associated with variable amplitude loading and other load history-dependent phenomena (e.g., period overloads) are an even longer term proposition.
- The design of methods to classify sources of uncertainty and stochasticity in modeling fatigue crack formation and MSC growth in 3D microstructures. These will have significant impact in modeling small crack arrest thresholds (i.e., fatigue limits) and considering multiaxial stress states, for example.
- Improved understanding and identification of volume element sizes and protocols for modeling and simulation, as well as nonlocal domain shapes and scales for averaging that correspond to fatigue mechanisms.
- Consideration of effects of point defects and ingress/diffusion of environmental species (e.g., oxygen, hydrogen) on fatigue crack formation and MSC growth.

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